CHEM 1035 – Lecture 24

Electron Configuration

The solution to Schrodinger's equation leads to descriptions of the energy "levels" for the hydrogen atom. Like the Bohr atom, solution of Schrodinger's equation for other atoms is not exact – they are, however, very good approximations. These approximate solutions are very similar to those of the hydrogen atom.

Light is shown to have either a wave description or a particle description. These principles can also be extended to particles, leading to a wave-particle duality of matte. The wave-particle duality of matter leads to the Quantum Mechanical description of atoms.

Quantum Numbers

Interger values that represent the Atomic Orbitals

- Principal Quantum Number (n)
- Angular Momentum Quantum Number (l)
- Magnetic Quantum Number (m_l)

1. Principle Quantum number (n), takes a positive integer value (1,2,3,…) This is representative of the relative size of the orbital. The greater the number, the further from the nucleus the probability contour extends.
2. Angular Momentum Quantum number (l), takes a value ranging from 0 to (n-1). This number is representative of the shape of the atomic orbital. If n = 0, then the orbital shape is spherical. If n = 1, then l can only be 0. If n = 3, then l = 0, 1, and 2. Note that the value of n limits the values available for l
3. Magnetic Quantum Number (m_l), this takes a value ranging from –l to +l. This represents the spatial orientation of the orbital. If n=1, then l=0 and m_l=0, this represents a sphere and the sphere is oriented equally distributed in all directions.

Examples of combinations of Quantum Numbers.

Energy levels, Orbital types,

Periodic Chart

Development attributed largely to Mendeleev, the elements in the periodic chart are arranged in groups (columns) containing elements with common physical and chemical properties. One of the great successes of Mendeleev's chart was that he was able to predict the existence of, and properties of elements that had not yet been discovered.

With solutions of Schrodinger's equation showing that all atoms have very similar atomic orbitals (with similar energies). These atomic orbitals are the "stationary states" that Bohr referred to.

The existence of similar energy atomic orbitals (which contain the electrons) begins to tell us why some atoms have similar chemical and physical properties.

The chemistry of atoms can be described as being due to formation or breaking of bonds. "Bonds" are the sharing/exchange of electrons. To understand chemistry, therefore, we need to examine the relationship between electrons and the atomic orbitals.

The 4th Quantum Number

- The previous 3 quantum numbers designate the atomic orbital
- The 4th quantum number describes a unique property of an electron that occupies an atomic orbital

The Electron-Spin Quantum Number

Electron-Spin Quantum Number, symbolized by m_s, and takes a value of +1/2 or -1/2. Each electron generates a tiny magnetic field. This magnetic field is attributed to the electron spinning. It is found that the spin of the electron is in one direction or the other (e.g. only 2 values of the Electron Spin QN are possible). The values of +/- ½ are due to the fact that for the Hydrogen atom it is found that ½ of the electrons have one spin, and the other ½ have the other spin.

With the 4 quantum numbers – 3 describing the atomic orbital, and the 4th characteristic of the electron – we have a a way of uniquely identifying each electron and its energy in any atom. That is, all atoms have a unique set of 4 quantum numbers.

What does this say about the number of electrons that can be in any one atomic orbital? There can only be 2 electrons in any given atomic orbital.

Pauli Exclusion Principle

No 2 electrons in the same atom can have the same 4 quantum numbers.

The Pauli exclusion principle provides a unique “Identifier” for each electron within a given atom. Examples: consider the He atom. What are the 4 QN for the 2 electrons.

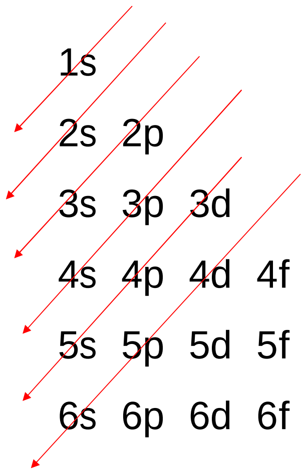
What does this say about how many electrons any one atomic orbital can contain?

Atomic "Ground" State

- The Ground state of an atom is the lowest energy atomic structure.

Because the Principle QN is representative of the energy of the atomic orbitals, it makes sense that electrons will occupy those orbitals with the lowest value of "n" first. After He, the elements begin to fill the n=2 shell. In this case, where do the next electrons go? 2s or 2p?

Atomic Orbital Relative Energies



Electrons fill the orbitals according to the available atomic orbitals with the lowest energy.

Why do the orbitals fill in this order?

The electrons fill the atomic orbitals according to their relative energies. We can get a sense of their relative energies by considering the attraction of the nucleus for the electrons.

- Orbitals that extend further from the nucleus have less energy because the electron has less attraction to the nucleus,
- Larger Charges have stronger attraction for each other.

These guidelines are Coulombs law for the interaction energy between opposite charges. Let's look to see how it applies to electrons. Consider the attraction between electrons and the nucleus and different atoms as we increase the Atomic number by 1, starting with Hydrogen.

Effect of charge? Shielding?

Aufbau Principle

The recurring pattern for filling available atomic orbitals in any atom is found by simply adding an electron to the available lowest energy atomic orbital.

This allows us to build up an “electron configuration” of the atom

Electron configuration – a shorthand notation that expresses the arrangment of the electrons in the “ground” state of the atom. It consists of the principal energy level (QN) the letter designation of the angular momentum QN to indicate the type of orbital the electron exists in (s, p, d, f), and the number of electrons contained in that sublevel.

Examples: H, He, Li, Be

Hund's Rule

When more than one sublevel of equal energy exists, then the electron configuration of lowest energy has the maximum number of unpaired electrons with parallel spins (e.g. same spin QN)

This says that the p_x, p_y, and p_z orbitals fill with one electron first before we begin to pair the electrons.

Examples: B, C, N, O, F, and Ne

Start on the 3rd row: Na, Mg, Al, Si, P, S – Notice anything about these electron configurations? The sequence begins to repeat itself.